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COMPUTED HEATS OF FORMATION

by

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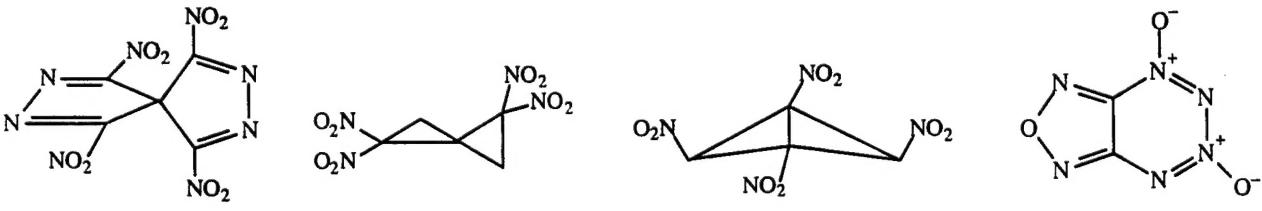
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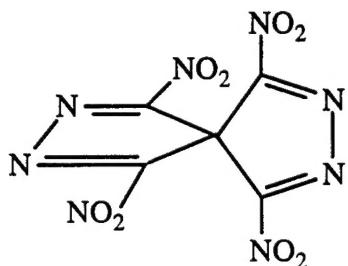
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13. ABSTRACT (Maximum 200 words) Computed heats of formation for 1 - 4.			
			
1	2	3	4
1: ΔH_f^{298K} (solid) = 157 kcal/mole = 524 cal/g	3: ΔH_f^{298K} (solid) = 59 kcal/mole = 250 cal/g		
2: ΔH_f^{298K} (solid) = 46 kcal/mole = 183 cal/g	4: ΔH_f^{298K} (solid) = 143 kcal/mole = 918 cal/g		
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We have used our density functional procedure [1] to compute the heats of formation of the compounds **1 - 4**, in response to a request from R. Naylor (Allegany Ballistics Laboratory). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the liquid and solid state values by subtracting, respectively, the heat of vaporization and the heat of sublimation. These are obtained by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [3,4].

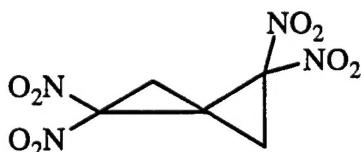
Results:

1



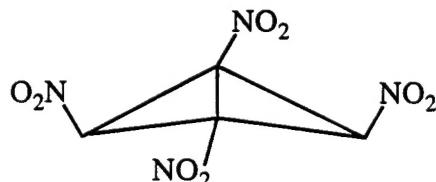
$$\begin{aligned}\Delta H_f^{298K} (\text{gas}) &= 189 \text{ kcal/mole} = 630 \text{ cal/g} \\ \Delta H_f^{298K} (\text{liquid}) &= 174 \text{ kcal/mole} = 579 \text{ cal/g} \\ \Delta H_f^{298K} (\text{solid}) &= 157 \text{ kcal/mole} = 524 \text{ cal/g}\end{aligned}$$

2



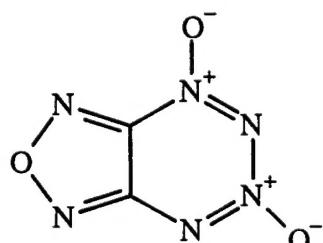
$$\begin{aligned}\Delta H_f^{298K} (\text{gas}) &= 76 \text{ kcal/mole} = 304 \text{ cal/g} \\ \Delta H_f^{298K} (\text{liquid}) &= 60 \text{ kcal/mole} = 243 \text{ cal/g} \\ \Delta H_f^{298K} (\text{solid}) &= 46 \text{ kcal/mole} = 183 \text{ cal/g}\end{aligned}$$

3



$$\begin{aligned}\Delta H_f^{298K} (\text{gas}) &= 85 \text{ kcal/mole} = 364 \text{ cal/g} \\ \Delta H_f^{298K} (\text{liquid}) &= 71 \text{ kcal/mole} = 303 \text{ cal/g} \\ \Delta H_f^{298K} (\text{solid}) &= 59 \text{ kcal/mole} = 250 \text{ cal/g}\end{aligned}$$

4



$$\begin{aligned}\Delta H_f^{298K} (\text{gas}) &= 165 \text{ kcal/mole} = 1058 \text{ cal/g} \\ \Delta H_f^{298K} (\text{liquid}) &= 152 \text{ kcal/mole} = 974 \text{ cal/g} \\ \Delta H_f^{298K} (\text{solid}) &= 143 \text{ kcal/mole} = 918 \text{ cal/g}\end{aligned}$$

For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [5,6].

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